Quantum electrodynamics of heavy ions and atoms

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Abstract

The present status of quantum electrodynamics (QED) theory of heavy few-electron ions is reviewed. The theoretical results are compared with available experimental data. A special attention is focused on tests of QED at strong fields and on determination of the fundamental constants. A recent progress on calculations of the QED corrections to the parity nonconserving 6s-7s transition amplitude in neutral Cs is also discussed.

1 Introduction

Basic principles of quantum electrodynamics (QED) were formulated to the beginning of 1930's as the result of merging quantum mechanics and special relativity. This theory provided description of such low-order processes as emission and absorption of photons and creation and annihilation of electron-positron pairs. However, application of this theory to calculations of some higher-order effects gave infinite results. This problem remained unsolved till the late of 1940's, when Lamb and Retherford discovered the $2p_{1/2} - 2s$ splitting in hydrogen, which is presently known as the Lamb shift. This discovery stimulated theorists to complete the creation of QED since it was believed that this splitting is of QED origin.

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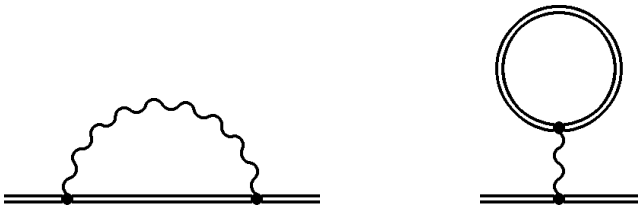
Figure 1: Self-energy (a) and vacuum-polarization (b) diagrams.



First evaluation of the Lamb shift was given by Bethe. The rigorous QED formalism was developed by Dyson, Feynman, Schwinger and Tomonaga. They found that all divergences can be removed from the theory by the renormalization procedure. All calculations in QED are based on the perturbation theory in a small parameter, which is the fine structure constant $\alpha \approx 1/137$. Individual terms of the perturbation series are conveniently represented by Feynman diagrams. For instance, the lowest-order contribution to the Lamb shift in a H-like atom is determined by so-called self-energy and vacuum-polarization diagrams, presented in Fig. 1.

Till the beginning of 1980's tests of quantum electrodynamics were mainly restricted to light atomic systems: hydrogen, helium, positronium, and muonium. In these systems, in addition to α, there is another small parameter, which is αZ (Z is the nuclear charge number). For this reason, calculations of light atoms were based on expansion in these two parameters. It means that with light atomic systems we can test QED only to few lowest orders in the parameters α and αZ. A unique opportunuty to study QED effects to all orders in αZ appeared in experiments with heavy few-electron ions, such as, for instance, H-like uranium or Li-like uranium. High-precision experiments with these ions became possible in the last two decades [1]. In heavy few-electron ions the number of electrons is much smaller than the nuclear charge number. For this reason, to the zeroth-order approximation, we can neglect the interelectronic interaction and consider that the electrons interact only with the Coulomb field of the nucleus. The interelectronic-interaction and QED effects are accounted for by perturbation theory in the parameters

$1/Z$ and α, respectively [2, 3]. For very heavy ions the parameter $1/Z$ becomes comparable with α and, therefore, all contributions can be classified by the parameter α. But, in contrast to light atoms, the parameter αZ is no longer small. It means that all calculations must be performed without any expansion in the parameter αZ.

2 Binding energy in heavy ions

2.1 H-like ions

To the zeroth-order approximation, a hydrogenlike ion is described by the Dirac equation with the Coulomb field of the nucleus ($\hbar = c = 1$):

$$(\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + V_{\rm C}(r))\psi(\mathbf{r}) = E\psi(\mathbf{r})\,. \tag{1}$$

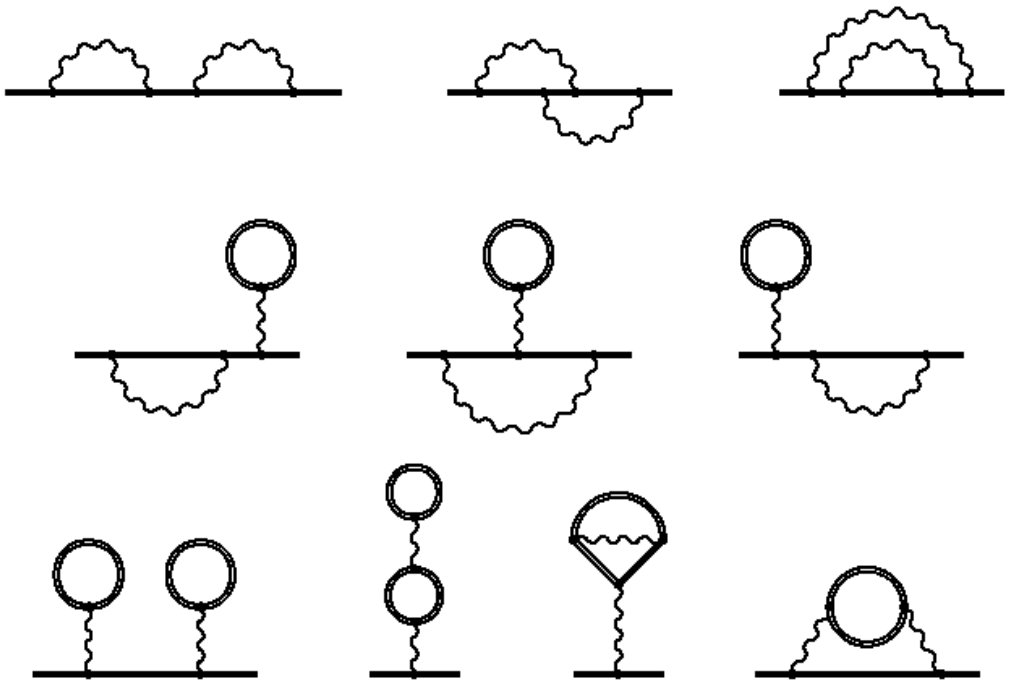
For the point-charge nucleus, $V_{\rm C}(r) = -\alpha Z/r$, this equation can be solved analytically (see, e.g., Refs. [2, 3]). To get the binding energy to a higher accuracy we need to evaluate quantum electrodynamic and nuclear corrections.

The finite-nuclear-size correction is evaluated by solving the Dirac equation with the potential induced by an extended nuclear charge-density distribution and taking the difference between the energies for the extended and point-charge nucleus. This can be done either numerically (see, e.g., Ref. [4]) or analytically [5]. In contrast to the nonrelativistic case, where the corresponding correction is completely defined by the root-mean-square nuclear radius $\langle r^2\rangle^{1/2}$, in heavy ions the higher-order moments of the nuclear charge distribution may affect the nuclear-size correction on a 1% accuracy level.

The QED corrections of first order in α are determined by the self-energy (SE) and vacuum-polarization (VP) diagrams (Fig. 1a,b). High-precision calculation of the SE diagram to all orders in αZ was performed by Mohr [6] while the VP diagram was first evaluated by Soff and Mohr [7] and by Manakov *et al.* [8]. Nowadays calculation of these diagrams causes no problem.

The QED corrections of second order in α are determined by diagrams depicted in Fig. 2. Most of these diagrams can be evaluated by adopting the methods developed for the first-order SE and VP corrections [2]. The most difficult task consists in evaluation of the SE-SE diagrams and the combined

Figure 2: Two-loop one-electron Feynman diagrams.



SE-VP diagrams presented in the last row of Fig. 2. The whole gauge-invariant set of the SE-SE diagrams was calculated in Ref. [9]. As to the combined SE-VP diagrams mentioned above, to date they have been evaluated only in the free-electron-loop approximation (see Ref. [2] and references therein).

Next, one should consider the nuclear recoil effect. It is known that in the nonrelativistic theory of a hydrogenlike atom the nuclear recoil effect can easily be taken into account using the reduced electron mass, $\mu = mM/(m+M)$, where M is the nuclear mass. But this is not the case in the relativistic theory. The full relativistic theory of the recoil effect can be formulated only in the framework of QED. For a hydrogenlike ion, a closed expression for the recoil effect to first order in m/M accounting for the complete αZ-dependence was derived in Ref. [10] (see also Ref. [11] and references therein). Numerical evaluation of this expression to all orders in αZ was performed in Ref. [12].

Finally, one should take into account the nuclear polarization correction, which sets the ultimate accuracy limit up to which QED can be tested with heavy ions. This correction is determined by the electron-nucleus interaction diagrams in which the intermediate nuclear states are excited. It was evaluated in Refs. [13, 14].

The individual contributions to the ground-state Lamb shift in $^{238}U^{91+}$, which is defined as the difference between the exact binding energy and the binding energy derived from the Dirac equation for the point-charge nucleus, are given in Table 1. The finite-nuclear-size correction is evaluated for the Fermi model of the nuclear charge distribution with $\langle r^2\rangle^{1/2} = 5.8507(72)$ fm [15]. The uncertainty of this correction is estimated by adding quadratically two errors, one obtained by varying the root-mean-square radius and the other obtained by changing the model of the nuclear-charge distribution from the Fermi to the homogeneously-charged-sphere model. According to the table, the present status of the theory and experiment on the ground-state Lamb shift in $^{238}U^{91+}$ provides a test of QED on the level of about 2%.

2.2 Li-like ions

To date, the highest accuracy was achieved in experiments with heavy Li-like ions [17, 18, 19]. In these systems, in addition to the one-electron contributions discussed above, one has to evaluate two- and three-electron contributions. To first order in α, the two-electron contribution is determined

Finite nuclear size	198.33(52)
QED of first order in α	266.45
QED of second order in α	-1.26(33)
Nuclear recoil	0.46
Nuclear polarization	-0.20(10)
Total theory	463.78(62)
Experiment [16]	460.2(4.6)

Table 1: Ground-state Lamb shift in $^{238}U^{91+}$, in eV.

by the one-photon exchange diagram whose calculation causes no problem. To second order in α, one should consider the two-photon exchange diagrams and the self-energy and vacuum-polarization screening diagrams. Accurate evaluations of these diagrams were accomplished by different groups [20]. In addition, to gain the required accuracy, we need to evaluate the interelectronic-interaction corrections of third order in the parameter $1/Z$. The corresponding evaluation within the Breit approximation was performed in Ref. [21].

The individual contributions to the $2p_{1/2} - 2s$ transition energy in Li-like uranium are presented in Table 2. The Breit approximation value indicates the transition energy which can be derived from the Breit equation. The QED contribution of second order in α incorporates a recent result for the two-loop SE contribution from Ref. [22]. The total theoretical value of the transition energy, 280.76(13) eV, agrees with the related experimental value, 280.645(15) eV [19]. Comparing the first- and second-order QED contributions with the total theoretical uncertainty, we conclude that the present status of the theory and experiment for Li-like uranium provides a test of QED on a 0.3% level to first order in α and on a 8% level to second order in α.

3 Hyperfine splitting in heavy ions

To date, there are several high-precision measurements of the hyperfine splitting (HFS) in heavy hydrogenlike ions [23, 24, 25, 26]. The hyperfine splitting of a hydrogenlike ion can be written as

$$\Delta E = \Delta E_{\rm Dirac}(1 - \varepsilon) + \Delta E_{\rm QED}\,, \tag{2}$$

Breit approximation	322.18(9)
QED of first order in α	-42.93
QED of second order in α	1.55(9)
Nuclear recoil	-0.07
Nuclear polarization	0.03(1)
Total theory	280.76(13)
Experiment [19]	280.645(15)

Table 2: The $2p_{1/2} - 2s$ transition energy in Li-like uranium, in eV.

where the Dirac value incorporates the relativistic and nuclear charge-distribution effects, ε is the nuclear magnetization distribution correction (so-called Bohr-Weisskopf effect), and $\Delta E_{\rm QED}$ is the QED correction. The most accurate calculations of the QED correction were performed in Refs. [27, 28]. The theoretical uncertainty is almost completely determined by the uncertainty of the Bohr-Weisskopf (BW) effect. Table 3 presents the ground-state hyperfine splitting in $^{209}Bi^{82+}$ obtained by different methods. The theoretical value based on the single-particle nuclear model [27] agrees well with the experiment [23] but has a rather large uncertainty. The most elaborated value obtained within a many-particle nuclear model [29] disagrees with the experiment. A semiempirical evaluation employing the experimental value for the HFS in muonic Bi [30] yields the value which deviates by 2σ from the experiment. Since the QED correction is comparable with the uncertainty due to the BW effect, it is rather difficult to test QED by the direct comparison of the theory and experiment on the hyperfine splitting in heavy H-like ions. However, it has been found that QED effects on the HFS can be tested by studying a specific difference of the ground-state HFS values in H- and Li-like ions of the same isotope [31]. Namely, it was shown that the difference

$$\Delta' E = \Delta E^{(2s)} - \xi \Delta E^{(1s)} \,, \tag{3}$$

where $\Delta E^{(1s)}$ and $\Delta E^{(2s)}$ are the HFS in H- and Li-like ions of the same isotope, is very stable with respect to variations of the nuclear model, if the parameter ξ is chosen to cancel the BW corrections in the right-hand side of equation (3). The parameter ξ is almost independent of the nuclear structure and, therefore, can be calculated to a high accuracy. In case of

Theory [27]	Theory [29]	Theory [30]	Experiment [23]
5.101(27)	5.111(-3,+20)(5)	5.098(7)	5.0840(8)

Table 3: Ground-state hyperfine splitting in $^{209}Bi^{82+}$, in eV.

Bi, the calculations yield $\xi = 0.16885$ and $\Delta' E = -61.27(4)$ meV. The non-QED and QED contributions amount to $-61.52(4)$ meV and 0.24(1) meV, respectively, and, therefore, the QED contribution is six times larger than the current total theoretical uncertainty. This method has a potential to test QED on level of a few percent, provided the HFS is measured to accuracy $\sim 10^{-6}$.

4 Bound-electron g-factor

The g-factor of an ion can be defined as the ratio of the magnetic moment of the ion to its mechanical moment, expressed in the Bohr magnetons. High-precision measurements of the g factor of H-like carbon [32] and oxygen [33] have triggered a great interest to related theoretical calculations (see Refs. [34, 35, 36] and references therein). In particular, these studies provided a new determination of the electron mass to an accuracy which is four times better than that of the previously accepted value [37]. An extension of the g-factor investigations to higher-Z ions could also lead to an independent determination of the fine structure constant α [38]. The accuracy of such a determination is, however, strongly limited by a large uncertainty of the nuclear structure effects which strongly increases when Z is growing [39]. In Ref. [40] it was shown that the ultimate accuracy limit can be significantly reduced in the difference

$$g' = g^{[(1s)^2(2s)^2 2p_{1/2}]} - \xi g^{[1s]}\,, \tag{4}$$

where $g^{[(1s)^2(2s)^2 2p_{1/2}]}$ and $g^{[1s]}$ denote the g-factors of $^{208}Pb^{77+}$ and $^{208}Pb^{81+}$, respectively. The parameter ξ must be chosen to cancel the nuclear size effect in this difference. In Ref. [40] it was shown that measurements of the g factor of B- and H-like lead to the same accuracy as for carbon, accompanied by the corresponding theoretical calculations, can provide a determination of α to a higher acuracy than that from the recent compillation by Mohr and Taylor

[37]. This method can also compete in accuracy with the new determination of α by Gabrielse and co-workers [41].

5 QED corrections to the $6s - 7s$ PNC transition amplitude in neutral ^{133}Cs

The $6s - 7s$ PNC transition amplitude in neutral ^{133}Cs [42] remains one of the most attractive subject for tests of the standard model (SM) at low energies. The measurement of this amplitude to a 0.3% accuracy [43] has stimulated theorists to improve the related calculations. These improvements, that included evaluations of the Breit interaction [44, 45], more precise calculations of the electron-correlation effects [46], and calculation of the vacuum-polarization part of the QED correction [47], gave the value for the weak charge of the cesium nucleus, which deviates by 2σ from the prediction of the standard model. This discrepancy urgently required calculations of the self-energy part of the QED correction. Evaluation of the whole gauge-invariant set of the SE corrections to the PNC transition amplitude with the Dirac-Fock wave functions was performed in Ref. [48]. The total result for the binding QED correction was found to amount to -0.27%. This value differs from the previous results for the total binding QED effect, $-0.5(1)\%$ [49] and $-0.43(4)\%$ [50]. The discrepency can be explained by some approximations made in the previos calculations. In particular, instead of calculating the QED corrections to the PNC amplitude, the previous papers were dealing with evaluation of the QED corrections to the PNC mixing coefficient which is a rather artificial subject for QED. However, a semiempirical revision of the previous results [51] gave a value for the QED correction which is very close to that of Ref. [48] .

Combining the QED correction with other theoretical contributions and comparing the total PNC amplitude with the experiment for an average value for the vector transition polarizabilty, $\beta = 26.99(5)a_{\rm B}^3$ (see Ref. [46] and references therein), one obtains for the weak charge of ^{133}Cs:

$$Q_W = -72.65(29)_{\rm exp}(36)_{\rm th}\,. \tag{5}$$

This value deviates from the SM prediction of $-73.19(13)$ [52] by 1.1 σ. Further progress on the PNC tests in ^{133}Cs can be achieved either by more accurate atomic structure calculations or by more precise measurements.

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